



## Supplement of

## A new machine-learning-based analysis for improving satellite-retrieved atmospheric composition data: OMI SO<sub>2</sub> as an example

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Figure S1: (a) Monthly mean analyzed SCDs for March 2005 using ReLU as the activation function in both hidden layers of the NNs. (b) The differences in the monthly mean analyzed SCDs for the same month between the NNs using ReLU as the activation function (in both hidden layers) and the original NNs (soft sign and sigmoid as the activation function for the first and second hidden layer, respectively). (c) The mean  $SO_2$  SCDs for 1-degree latitude bands from the two NN architectures over generally clean areas (monthly mean SRR < 3).



Figure S2: Monthly mean SO<sub>2</sub> SCDs for March 2005 from (first column) the original PCA retrievals and (second column) the neural network based analysis, and (third column) their differences for (a-c) January, (d-f) April, (g-i) July and (j-l) October 2005.



Figure S3: Same as Figure 6 but for India. For polluted areas ( $SCD_{NN} > 0.15 \text{ DU}$ ), the mean relative difference between the original and analyzed SO<sub>2</sub> SCDs is 9%, with the original being greater.



Figure S4: Same as Figure 6 but for the Middle East. For polluted areas ( $SCD_{NN} > 0.15 \text{ DU}$ ), the mean relative difference between the original and analyzed SO<sub>2</sub> SCDs is 14%, with the original being greater.



Figure S5: Same as Figure 6 but for South Africa. For polluted areas ( $SCD_{NN} > 0.15 \text{ DU}$ ), the mean relative difference between the original and analyzed SO<sub>2</sub> SCDs is -1%, with the original being smaller.



Figure S6: Same as Figure 6 but for the eastern U.S. For polluted areas (SCD<sub>NN</sub> > 0.15 DU), the mean relative difference between the original and analyzed SO<sub>2</sub> SCDs is -11%, with the original being smaller.



Figure S7: Same as Figure 6 but for Norilsk, Russia. For polluted areas (SCD<sub>NN</sub> > 0.5 DU), the mean relative difference between the original and analyzed SO<sub>2</sub> SCDs is -4%, with the original being smaller.



Figure S8: Same as Figure 6 but for the southeast Pacific for October 2005. The large SO<sub>2</sub> plume is from the 2005 Sierra Negra eruption that started on October 22. For pixels with relatively large SO<sub>2</sub> loading (SCD<sub>NN</sub> > 1 DU), the mean relative difference between the original and analyzed SO<sub>2</sub> SCDs is 20%, with the original being greater.



Figure S9. The (a) original, (b) NN analysed OMI SO<sub>2</sub> SCDs and (c) their differences for March 2005 for pixels with SCD/RMS ratios (SRR<sub>i</sub>)  $< \overline{SRR}$ , where  $\overline{SRR}$  represents the monthly median of the daily mean SRRs calculated for each 3° latitude band.



Figure S10. Same as Figure S9 but for pixels with  $\overline{SRR} < SRR_i < \overline{SRR} + \sigma_{SRR}$ , where  $\sigma_{SRR}$  is the monthly median of the standard deviation of SRRs calculated daily for each 3° latitude band.





Figure S11. Same as Figure S9 but for pixels with  $\overline{SRR} + \sigma_{SRR} < SRR_i < \overline{SRR} + 2\sigma_{SRR}$ .





Figure S12. Same as Figure S9 but for pixels with  $\overline{SRR} + 2\sigma_{SRR} < SRR_i < \overline{SRR} + 3\sigma_{SRR}$ .

(a) Original:  $SRR_i > SRR + 3.0\sigma_{SRR}$ 



Figure S13. Same as Figure S9 but for pixels with SRR<sub>i</sub> >  $\overline{SRR}$  +  $3\sigma_{SRR}$ .